We claim:

1. A composition comprising a Staphylococcus undecaprenyl pyrophosphate synthase in crystalline form, said synthase comprising an amino acid sequence at least about 80% homologous to SEQ ID NO:1.

2. The composition of claim 1 wherein said synthase comprises an amino acid sequence at least about 95% homologous to SEQ ID NO:1

3. The composition of claim 1 wherein the molecules of said synthase have atomic coordinates according to Figure 5.

4. The composition of claim 1 wherein said synthase comprises at least one ligand.

5. The composition of claim 4 wherein the ligand is selected from the group consisting of farnesyl pyrophosphate, (S)-farnesyl thiopyrophosphate, isoprenyl pyrophosphate, magnesium ion, and sulfate ion.

6. The composition of claim 1 wherein said synthase comprises a first ligand binding site including the amino acid residues selected from the group consisting of Asp^{33}, Gly^{34}, Gly^{36}, Arg^{37}, Arg^{46}, Ala^{76}, Arg^{84}, Leu^{95}, Pro^{96}, and Phe^{148}.

7. The composition of claim 1 wherein the synthase comprises a first ligand binding site defined by amino acid residues Asp^{33}, Gly^{34}, Gly^{36}, Arg^{37}, Arg^{46}, Ala^{76}, Arg^{84}, Leu^{95}, Pro^{96}, and Phe^{148} having atoms having atomic coordinates according to Figure 5.

8. The composition of claim 1 wherein said synthase comprises a second ligand binding site including the amino acid residues selected from the group consisting of Asp^{33}, Arg^{201}, Arg^{207}, Ser^{209}, Glu^{220}(B), and Gly^{251}(B).

9. The composition of claim 1 wherein the synthase comprises a second ligand binding site defined by amino acid residues Asp^{33}, Arg^{201}, Arg^{207}, Ser^{209}, Glu^{220}(B), and Gly^{251}(B) having atoms having atomic coordinates according to Figure 5.

10. A method of identifying a potential ligand for an undecaprenyl pyrophosphate synthase, comprising:

(a) using a three-dimensional structure of said synthase as defined by at least atomic coordinates of amino acid residues 33, 34, 36, 37, 46, 76, 84, 95, 96, and 148 according to Figure 5;

(b) employing said three-dimensional structure to design or select said potential ligand;

(c) obtaining said potential ligand; and

(d) contacting said potential ligand with said synthase to determine binding of said potential ligand to said synthase.

11. The method of claim 10 wherein step (c) precedes step (b).

12. A method for identifying a potential inhibitor of a mutant undecaprenyl pyrophosphate synthase, said method comprising:

(a) using a three-dimensional structure of a known undecaprenyl pyrophosphate synthase as defined by atomic coordinates of said known synthase according to Figure 5;

(b) replacing one or more amino acids of said known synthase, said amino acids selected from 33, 34, 36, 37, 46, 76, 84, 95, 96, 148, 201, 207, 209, 220, and 251 of SEQ ID NO:1, with a different naturally occurring amino acid, thereby forming said mutant synthase;

(c) employing said three-dimensional structure to design or select said potential inhibitor; and

(d) contacting said potential inhibitor with said mutant synthase, optionally in the presence of a substrate, to test the ability of said potential inhibitor to inhibit said mutant synthase.

13. A method of identifying a ligand capable of binding to an undecaprenyl pyrophosphate synthase substrate binding site, said method comprising:

(a) introducing into a suitable computer program information defining said binding site, said information comprising atomic coordinates of amino acids capable of binding to a synthase substrate, wherein said program displays the three-dimensional structure of said binding site;

(b) creating a three dimensional model of a test compound in the computer program;

(c) docking said model of said test compound to the structure of said binding site;

(d) comparing the docking of said model of said test compound to the docking of known ligands of said synthase to provide an output of the program.

14. A method for identifying a potential inhibitor for an undecaprenyl pyrophosphate synthase, said method comprising:

(a) using a three-dimensional structure of said synthase as defined by atomic coordinates of said synthase according to Figure 5;

(b) employing said three-dimensional structure to design or select said potential inhibitor; and

(c) contacting said potential inhibitor with said synthase in the presence of a substrate to determine the ability of said potential inhibitor to inhibit said synthase.

15. A method of drug design comprising using atomic coordinates of a Staphylococcus undecaprenyl pyrophosphate synthase having at least one ligand binding site to computationally evaluate relative associations of chemical entities with the ligand binding site and produce an output.

16. A method for solving a crystal form comprising using atomic coordinates of a Staphylococcus undecaprenyl pyrophosphate synthase crystal or portions thereof, to solve a crystal form of a mutant, homolog or co-complex of the undecaprenyl pyrophosphate synthase by molecular replacement.

17. A machine-readable data storage medium comprising a data storage material encoded with machine-readable data comprising atomic coordinates comprising amino acid residues 33, 34, 36, 37, 46, 76, 84, 95, 96, and 148 according to Figure 5.

18. The machine-readable data storage medium of claim 17 wherein said machine-readable data further comprises atomic coordinates comprising at least one amino acid residue selected from the group consisting of 201, 207, 209, 220(B), and 251(B) according to Figure 5.

19. A computer-implemented tool for design of a drug, comprising:

(a) a three-dimensional structure of an undecaprenyl pyrophosphate synthase as defined by atomic coordinates of Figure 5;

(b) a model of a chemical entity; and

(c) a computer program addressing said coordinates and capable of modeling the docking of said chemical entity in a ligand binding site of said three-dimensional structure to produce an output.

20. A computer for producing a three-dimensional representation of an undecaprenyl pyrophosphate synthase ligand binding site, said computer comprising:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data comprising the atomic coordinates comprising the amino acid residues 33, 34, 36, 37, 46, 76, 84, 95, 96, and 148 according to Figure 5;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.